

$$T_n = T_L [e^{\phi/V_T} u]^{-5/4} g_n; \quad T_p = T_L [e^{-\phi/V_T} v]^{-5/4} g_p$$

A new Scharfetter-Gummel-type discretization was developed for each of the transformed linear HD equations. The SG discretization yields a discrete system with coefficient matrices which are well conditioned, thereby helping to avoid numerical problems associated with their solution. The coordinated use of the new variables, the Gummel iterative approach, and the SG discretization yields a robust approach to solving the HD equations. We demonstrate the new approach by applying it to a realistic 0.35 μm 2-D LDD MOSFET structure. The following page gives some example results including the predicted LDD device I-V characteristics.

P29. Modelling of Hot Acoustic Phonon Propagation in Two Dimensional Layers, N. A. Bannov, V. V. Mitin, and F. T. Vasko, Department of Electrical and Computer Engineering, Wayne State University, Detroit, MI 48202. Acoustic modes in layered structures differ substantially from modes in bulk material. We have obtained the quantum kinetic equation for confined acoustic phonons interacting with 2D electron gas and solved it for the case of phonon transport in a layered structure. We use the Wigner distribution function, $N_m(\mathbf{q}_{\parallel}, r_{\parallel})$, to describe the phonon sub-system; here m is a discrete index for mode number, q_{\parallel} and r_{\parallel} are the in-plane phonon wave vector and coordinate. The kinetic equation for $N_m(\mathbf{q}_{\parallel}, r_{\parallel})$, have the following form

$$\left(\frac{\partial}{\partial t} + S_{m,q} \frac{\partial}{\partial r_{\parallel}} \right) N_m(q_{\parallel}, r_{\parallel}) = T_m(q_{\parallel}, r_{\parallel}), \text{ where } S_{m,q} \text{ is the renormalised due to electron-phonon interactions}$$

phonon group velocity, $T_m(q_{\parallel}, r_{\parallel})$ is a collision integral responsible for decay of phonon modes. We have obtained explicit expressions for $T_m(q_{\parallel}, r_{\parallel})$ and $S_{m,q}$ for the case of a deformation potential interaction of 2D phonons with 2D electrons. The renormalization of the acoustic wave velocity and characteristic decay time have substantially different dependence on m and q_{\parallel} for $aq_{\parallel} \ll 1$ and for $aq_{\parallel} \gg 1$, where a is a width of the quantum well. We have numerically solved the kinetic equation for the thermal pulse propagation along a layer. Due to existence of several confined acoustic modes in layered structures, and complicated dispersion relation for confined phonons, the arrival time for different phonons varies significantly. This fact may be used for probing electron-phonon interaction in layered structures by time-of-flight technique.

P30. Numerical Simulation of Heat Removal from Low Dimensional Nanostructures, V. V. Mitin, N. A. Bannov, R. Mickevicius, and G. Paulavicius, Department of Electrical and Computer Engineering, Wayne State University, Detroit, MI 48202. Heat removal from active elements of high performance ultralarge integrated circuits is one of the major technical problems in developing new generations of IC. We have investigated the acoustic phonon radiation due to electron-acoustic phonon interaction in double barrier quantum wells and quantum wires. The electron and phonon density matrices are governed by coupled kinetic equations which have been solved numerically by the Monte Carlo technique. The effect of hot electrons on the radiation pattern of emitted phonons has been taken into account. We have calculated the angular and energy spectrum of nonequilibrium acoustic phonons radiated from low dimensional structures. A major peculiarity of acoustic phonon emission is a violation of the conservation law for the phonon wave vector component which is perpendicular to the direction of spatial confinement. Due to this violation the characteristic energies of the emitted acoustic phonons greatly exceed the energies of acoustic phonons emitted in bulk materials and are order of several meV . Nevertheless, such phonons propagate ballistically over macroscopic distances and have been detected experimentally. Except for the case of a strongly degenerate electron gas, the along-structure wave vectors of acoustic phonons emitted by electrons in nanostructures are smaller than the transverse wave vectors. Therefore the acoustic phonons carry energy primary in the direction normal to the nanostructure. We have demonstrated that due to large acoustic-phonon energies and strong scattering in nanostructures the heat removal by ballistic fluxes of acoustic phonons is extremely efficient.

P31. A Hot-Hole Transport Model Based on Spherical Harmonics Expansion of the Anisotropic Bandstructure, M. Harrer, H. Kosina, Institute for Microelectronics, Vienna Technical University,

Gusshausstrasse 27-29, A-1040 Vienna, Austria. Monte Carlo transport simulations call for effective methods to calculate the free flight duration and to choose the scattering mechanism and the state after scattering. We propose a representation of the valence bands using an expansion into a series of spherical harmonics that is capable of resolving details of the band structure both at the center and at the boundary of the Brillouin zone. The basic intention of our method is to simplify the calculation of the integrated scattering probability. Assume that the energy-wave-vector relationship is given in polar coordinates: $\varepsilon = E(k, \Omega)$. Here, ε is the energy of the hole, k the magnitude of the wave vector, and Ω denotes (θ, ϕ) . We now introduce a coordinate transformation $(k, \Omega) \rightarrow (\varepsilon, \Omega)$, which transforms k to ε and lets Ω unchanged: $k = K(\varepsilon, \Omega)$. For any given Ω the function K is defined to be the inverse of the function E . The function K can be interpreted to describe the shape of an equi-energy surface in \mathbf{k} -space. Inversion of a function is possible only in an interval where the function is monotonous. By inspection of the full band structure one finds that both the heavy hole and the split-off bands can entirely be represented by such functions K . Above a hole energy of $E_x(3.04\text{eV})$ inversion of the light hole band is no longer unique. In this work, we represent the function K as a series of spherical harmonics.

$$K_b(\varepsilon, \Omega)^3 = \frac{3}{4\pi} \sum_{l=0}^{\infty} \sum_{m=0}^l a_{lm}^b(\varepsilon) P_l^m(\cos\theta) T_m(\cos\phi), \quad b=H,L,SO. \quad (1)$$

Derivation of the scattering rates is considerably eased by taking the third power of K as the function to be expanded. For symmetry reasons non-vanishing coefficients only exist for even values of l and m being a multiple of 4. With (1) a set of functions $a_{lm}^b(\varepsilon)$ contains the whole band structure information. The essential advantage of the spherical harmonic expansion of the valence band is the resulting representations of the total scattering rates and of the distribution of the scattering angle. Our transport model accounts for three different scattering mechanisms, namely acoustic deformation potential (ADP) scattering in the elastic approximation, optical deformation potential (ODP) scattering and ionized impurity scattering (ION) in the Brooks and Herring formalism. The angular distribution functions of the solid angle after scattering are also given by spherical harmonics series. The rejection technique is used to choose the after scattering state. The free flight time is calculated by a self-scattering method. The functions $a_{lm}^b(\varepsilon)$ are represented numerically by means of a finite element method. The free parameters of the series are determined by a variational approach. The number of harmonics was made a function of energy ranging from $l_{\max} = 20$ at lower energies to $l_{\max} = 60$ at higher energies. In this work the steady-state hole transport in silicon has been simulated using the expansion (1) for the heavy and light hole bands up to a hole energy of $E_{\text{hole}} = 3.04\text{eV}$. The split-off band has been neglected. Figure (1) shows the numerical band structure compared with the series representation. The numerical band structure has been computed by a nonlocal empirical pseudopotential method. Figure (2) depicts the resulting drift velocities in comparison to measured data and Figure (3) the simulated average hole energy, both as a function of the electric field applied in characteristic directions.

P32. An Improved Ionized Impurity Scattering Model for Monte Carlo Calculations, *G. Kaiblinger-Grujin and H. Kosina, Institute for Microelectronics, Vienna Technical University, Gusshausstrasse 27-29, A-1040 Vienna, Austria.* We have developed a physically based ionized impurity scattering model including the following corrections to the standard Brooks-Herring model. First, momentum dependent screening of impurities by conduction electrons is taken into account assuming degenerate statistics. Second, the effect of multi-ion-scattering is included. Dynamical screening is described by a function of both the transferred momentum q and the Fermi level [1]. Unfortunately, this function is represented by an integral which cannot be solved analytically. We approximated this integral by an analytical expression which has exactly the same behavior as the original integral for large q and is a very good approximation for small q for arbitrary degeneration. The advantage of this approach is that we are able to get a closed form for the scattering rate without changing the physics of the underlying problem. With higher doping, the average distance between impurities becomes smaller and the neighboring ion potentials overlap appreciably, so that the single-site-model for ionized impurity scattering breaks down. Therefore it is necessary to consider scattering processes at two ion potentials simultaneously. Equally charged pairs of impurities scatter up to twice as effectively than monopoles [2]. The well-known problem of very large scattering rates at small angles is commonly solved by using a method after Ridley [3], which essentially cuts off the scattering rates at small